2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester

13533-05-6 | DTXSID5050397

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.59e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.92e-01

Confidence level: 8.69e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl acrylate
Measured: 1.60e-11
Predicted: 1.75e-11

Image not found
2-Ethoxyethyl methacrylate
Measured: 2.80e-11
Predicted: 2.95e-11

Image not found
4-Pentenyl acetate
Measured: 4.34e-11
Predicted: 4.13e-11

Image not found
Methyl methacrylate
Measured: 2.60e-11
Predicted: 2.84e-11

Image not found
Allyl acetate
Measured: 2.71e-11
Predicted: 2.97e-11